Multi-objective optimisation of flavour and processing time in beer fermentation via dynamic simulation

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Multi-objective Optimisation of Flavour and Processing Time in Beer Fermentation via Dynamic Simulation

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Abstract

Fermentation is an essential step in beer brewing: when yeast is added to hopped wort, sugars ferment into ethanol and higher alcohols. Progression is highly sensitive to the temperature manipulation invoked, influencing batch time and product quality. A novel computational implementation of a published kinetic model has been produced, rapidly generating temperature manipulations and simulating the operation of each candidate profile. Ethanol and key harmful by-product (diacetyl, ethyl acetate) concentrations are monitored in order to minimize fermentation time while ensuring product quality is maintained. Visualisation of the entire operational envelope clearly illustrates Pareto fronts and trade-offs among these design objectives. Comparing these simulation results with those of an industrial operational profile reveals that batch time can be reduced by as much as 15 hours when an acceptable sacrifice is made to by-product concentrations.

Keywords: Multi-objective optimisation, dynamic simulation, flavour, beer fermentation

1. Introduction

The production of beer is well documented, with suggestions that it is one of the world's oldest prepared beverages, dating back to the early Neolithic period (Arnold, 1911). Today beer is the most widely consumed alcoholic beverage in the world (Rehm et al., 2003) with the global beer market estimated to be over 500 billion USD in 2015 (Markets, 2013). Market competitiveness makes it imperative that brewers operate their production processes effectively: the ability to improve or optimise any stage of production will significantly affect profitability and the ultimate success or failure of a brewery. While many variations of the beer manufacturing process exist, industrial production almost invariably follows the scheme outlined in Fig. 1. Beer production is a complex chemical process: nevertheless, its only prerequisite is the incorporation of the same four essential ingredients: a starch source, yeast, hops and water (Southby, 1885).

2. The Fermentation Process

Fermentation is an essential brewing process unit operation, responsible for the alcohol content and characteristic taste of the final beer product. Yeast is introduced (pitching) to the cooled wort (a sugar-rich liquid intermediate) as it enters the fermentation vessels.

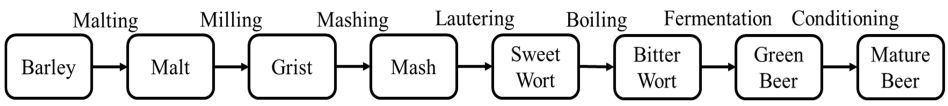


Figure 1. Block flow diagram of the beer production process.

The primary chemical reaction pathway is the conversion of sugars into ethanol and carbon dioxide, which is coupled with biomass growth and heat generation from the exothermic reaction. Concurrently, a range of species are formed at low concentrations by a multitude of side reactions, many of which impact product flavour considerably.

As system temperature strongly affects yeast growth and metabolic rate, brewers continually control the temperature inside the fermenter as the batch progresses. This aims to accelerate fermentation while ensuring yeast is not excessively denatured and flavour contributing by-product species are not produced in quantities which would impair product flavour. As such, a primary concern of the brewing industry is the selection and implementation of an appropriate dynamic temperate profile throughout the fermentation process, to ensure a high product quality, eliminate batch variations and to ensure brand consistency and customer satisfaction. It is common for steel fermenters to be equipped only with vessel cooling utilities, meaning that the temperature increase is induced only by the exothermic nature of key reaction pathways.

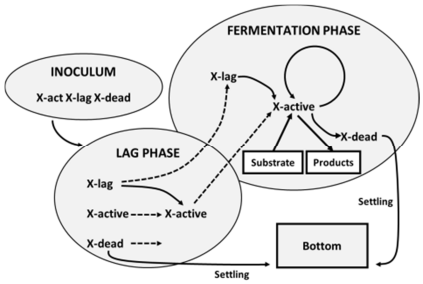
Fermentation has the longest duration of all stages in beer production, thus constituting the system bottleneck. To increase plant throughput and profitability, debottlenecking strategies are highly lucrative: avoiding the sizeable capital investment to increase the number of available vessels is preferable, so an investigation into batch time minimisation by modifying the fermentation temperature profile has been performed.

3. Reduced-order Fermentation Modelling

Historically, beer production has been based on proven recipes, obtained by altering the process with trial and error to achieve a more desirable product. Computational prediction and performance assessment of a biochemical process toward process optimisation requires a mathematical model representing species consumption and production. While beer brewing is an established industry, the system complexity and the numerous (over 600) species present (Vanderhaegen et al., 2006) induces a lack of understanding of much of the chemical phenomena taking place, making it extremely challenging to explicitly predict the effect of process alterations on the required processing time and product composition. Authors of previous studies postulated reduced-order dynamic fermentation models by considering only the key chemical reaction pathways, using parameters computed from their experimental campaign data.

3.1. Published Kinetic Models

The earliest work (Engasser et al., 1981) was based on fundamental pathways and the manner in which the evolution of alcohol and sugars depends on total biomass (yeast) concentration via Monod kinetics. Gee and Ramirez (1988) adapted this work to include temperature effects on rate expressions, and later revisited the model to consider further compounds (1994). Trelea at al. (2001) developed a fermentation model based on CO_2 production as sugar uptake and biomass growth cannot be readily measured online. Ethanol, yeast production and sugar consumption are related to CO_2 concentration with temperature dependent yield factors: three distinct model forms are considered, each with varying knowledge of the underlying biochemical phenomena. De Andrés-Toro et al. (1998) proposed an alternative kinetic model for beer production under industrial operating conditions, relying on predicting yeast evolution in order to subsequently compute chemical species growth. The model is appropriate for study due to its parameter determination and model validation taking place on an industrial scale, its inclusion of flavour degrading compounds and the wide valid temperate range (8-24 ºC).



$$\frac{dX_A}{dt} = \mu_x \cdot X_A - \mu_{DT} \cdot X_A + \mu_L \cdot X_L \quad (1)$$

$$\frac{dX_D}{dt} = -\mu_{SD} \cdot X_{dead} + \mu_{DT} \cdot X_A \quad (2)$$

$$\frac{dC_S}{dt} = -\mu_S \cdot X_A \quad (3)$$

$$\frac{dC_E}{dt} = f \cdot \mu_e \cdot X_A \quad (4)$$

$$\frac{dC_{EA}}{dt} = Y_{EA} \cdot \mu_x \cdot X_A \quad (5)$$

$$\frac{dC_{DY}}{dt} = \mu_{DY} \cdot C_S \cdot X_A - \mu_{AB} \cdot C_{DY} \cdot C_E \quad (6)$$

$$\frac{dX_l}{dt} = -\mu_L \cdot X_L \quad (7)$$

$$\mu_x = \frac{\mu_{x_0} \cdot C_s}{k_x + C_e} \quad (8)$$

$$\mu_{SD} = \frac{\mu_{SD_0} \cdot 0.5 \cdot C_{s_0}}{0.5 \cdot C_{s_0} + C_e} \quad (9)$$

$$\mu_s = \frac{\mu_{s_0} \cdot C_s}{k_s + C_s} \quad (10)$$

$$\mu_e = \frac{\mu_{e_0} \cdot C_s}{k_e + C_s} \quad (11)$$

$$f = 1 - \frac{C_e}{0.5 \cdot C_{s_0}} \quad (12)$$

Figure 2. Model for dynamic simulation of beer fermentation (de Andrés-Toro, 1998).

4. Model Description

The de Andrés-Toro model chosen for study considers five responses: ethanol (C_E), sugar (C_S), biomass (X_i) and two flavour-contributing compounds: diacetyl (C_{DY}) and ethyl acetate (C_{EA}). The single sugar compound represents the sum of all sugars present in the wort. Here the suspended biomass is distinguished into three forms: active (X_A), latent (X_L) and dead (X_D) cells. Active cells can promote fermentation, and duplicate and grow over time; however a portion of them will die and no longer contribute to fermentation, settling at the bottom of the vessel. Latent (lag) cells are unable to promote fermentation, but over time they are transformed into active cells, responsible for consumption of the fermentable material in the wort. A schematic diagram of the model process scheme, and the corresponding kinetic rate equations are presented in Fig. 2. Arrhenius growth rates (μ_i) are used to describe species progression, along with a stoichiometric yield factor (Y) and an inhibition factor on ethanol production (f).

5. Dynamic Simulation

The algorithm developed performs computation of dynamic chemical species profiles following any input temperature profile. Arrhenius parameter values are taken from the original model publication, excluding the diacetyl appearance and disappearance rates which are taken from subsequent work (Carillo-Ureta, 2001) due to the erratic profiles produced by the original formulation. Throughout all simulations initial biomass and sugar concentrations are assumed constant as 4 and 130 g L^{-1} respectively, such that the only factor influencing beer fermentation performance is the temperature manipulation profile employed. The code produced has been validated by comparing species profile predictions with those from literature (Carrillo-Ureta et al., 2001; Xiao et al., 2004) when following equivalent temperature manipulations. This model implementation has been used to predict the species progression when following the dynamic temperature manipulation from WEST Brewery, UK, the results of which are presented in Figure 3.

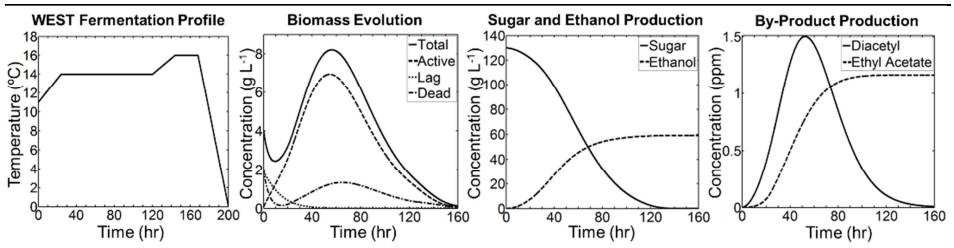


Figure 3. Dynamic model concentration predictions for industrial beer fermentation.

6. Multi-objective Optimisation

To assess the potential for process improvement versus current plant operation at WEST Brewery, Glasgow, UK an algorithm has been developed to rapidly generate plausible temperature manipulations which adhere to realistic operability constraints at a suitable level of temporal domain discretisation. In order to generate new manipulations, the dynamic temperature domain must be defined and discretised. The domain limits used here are given by Eqs. (13-14): to maintain the realistic operability window. Given the achievable temperature variation and control within an industrial scale fermentation vessel it is deemed appropriate to discretise the domain per 20 hour interval and per degree Celsius, where temperature profiles are formed by linear segments connecting these points. Across the 160 hour timespan this would inherently produce a vast number of unrealistic and undesirable profiles so a constraint is applied (Eqs. 15-16), removing those which evidently would produce poor performance, by not permitting temperature decrease/increase in the first and second halves of the process respectively.

$$0 < t < 160 \text{ (hr)} \qquad (13)$$

$$9 < T < 16 \text{ (ºC)} \qquad (14)$$

$$T(t_{n+1}) \geq T(t_n), \quad \text{for } t < \frac{t_{max}}{2} \qquad (15)$$

$$T(t_n) \geq T(t_{n+1}), \quad \text{for } t \geq \frac{t_{max}}{2} \qquad (16)$$

The temperature and time limits, discretisation level and constraints considered in the present study produce 175,252 unique temperature profiles. Simulating dynamic species evolution for the entire set of manipulations requires 3 hour of total processing time on an Intel Core ™ i7-4790. Key performance indicator data is plotted alongside the results of the actual industrial plant operating profile, represented by the hollow circular marker on the scatter plots (Figure 4). These results show vast performance variation between cases, emphasising the requirement for correct profile selection and implementation.

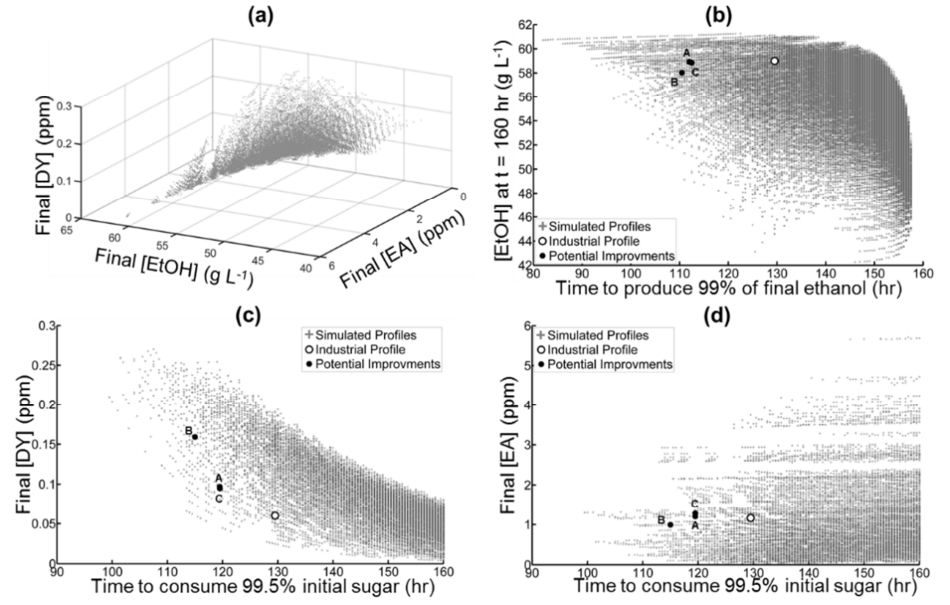


Figure 4. Product concentrations attainable envelope and operational map projections.

Fig. 4a shows the relationship between final product compound concentrations (attainable concentration envelope): it can be seen that the greatest ethanol production also corresponds to the highest production of undesirable by-products, well exceeding the taste threshold. It also indicates that a small sacrifice in final ethanol concentration can lead to large reductions in the concentrations of by-product compounds. Given the inherent trade-offs which exist, it is found that no case simulated can improve on each target (batch time and by-product reduction and ethanol production) simultaneously.

Fig. 4b depicts ethanol generation's relationship with processing time. It is revealed that WEST Brewery's operation falls in the acceptable region: it is significant that a vast family of solutions exist which simultaneously reduce fermentation time and increase ethanol concentration relative to this, shown in the upper leftmost corner of the figure.

Batch time and the corresponding by-product production is also considered. Fig. 4c illustrates that a reduction in batch time is associated with an increase in the product diacetyl concentration. The current industrial plant manipulation is producing a low ethyl acetate concentration given its batch time (t = 130 hours), close to the Pareto front of this plot which follows the minimum concentration boundary for any fermentation time. Diacetyl concentration is the most challenging variable to reduce without suffering a detrimental effect on other process parameters, given its proximity to this front. As it is below the levels produced by many fermentations, allowing diacetyl concentration to increase within acceptable limits is a valid strategy to reduce batch time.

Conversely, Fig. 4d shows that such a high fidelity correlation between ethyl acetate and batch time does not exist. Simulation data points are widely scattered, however it is found that longer batch times can coincide with higher ethyl acetate levels, while shortest batch times correspond to lower levels. The current industrial manipulation produces approximately the average ethyl acetate concentration for all fermentations of this duration: scope for reduction does exist, however the current value is not above the threshold where flavour would is negatively impacted meaning this is not a priority.

7. Temperature Manipulation: Operational Improvements

Of the scenarios simulated, three promising process improvements are suggested in Fig. 5: the performance of each is compared to industrial operation in Table 1. The results from each of these profiles is also highlighted in Fig. 4(b-d) with solid circular markers, allowing the performance of each profile to be readily visualized. A sizable batch time reduction is demonstrated in each case, with a minimal impact on the product quality.

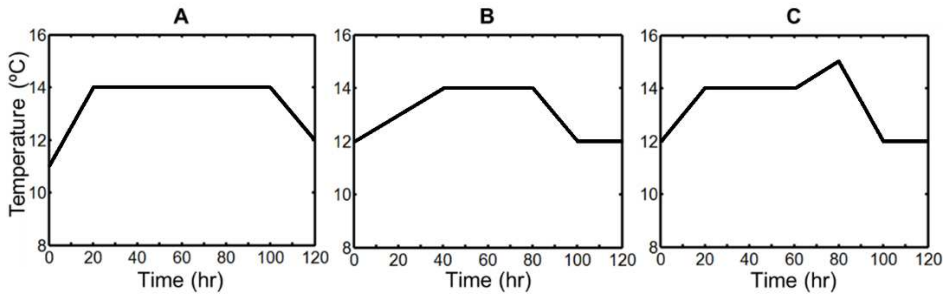


Figure 5. Dynamic temperature manipulation profiles inducing process improvement.

Table 1. Proposed fermentation improvements: effect on key beer flavour attributes.

		Industrial manipulation	Operational improvements		
			A	**B**	**C**
Fermentation time	hrs	129.5	119.5	115.0	119.5
Ethanol concentration	g L^{-1}	59.0	58.9	58.0	58.9
EA concentration	ppm	1.16	1.19	0.99	1.28
DY concentration	ppm	0.06	0.10	0.16	0.09

Options A and C show similar performance, a 10-hour reduction in fermentation time, with a small (0.1 g L^{-1}) reduction in product ethanol concentration and a marginal increase in both by-product compound concentrations. Option B may be preferable if a more significant decrease in ethanol concentration is permitted; a sacrifice of 1 g L^{-1} can reduce batch time by 15 hours, while reducing the ethyl acetate concentration by 15 %. The product diacetyl concentration is also increased as a result, however it is still well within tolerable limits, as there is no discernible flavour effect below 0.2 ppm (WEST). Thus we have demonstrated that depending on a brewer's particular product targets numerous dynamic simulations performed in this study represent viable strategies to reduce batch time, a clear benefit attainable by sacrificing low-priority process targets.

8. Conclusions

An algorithm has been developed to generate temperature manipulations which adhere to suitable operability constraints at an appropriate level of temporal domain discretisation. Simulation of each plausible scenario produces an array of potentially more suitable temperature manipulations, where small sacrifices in by-product (diacetyl or ethyl acetate) concentrations allow batch time to be reduced by up to 15 hours. This represents a substantial decrease in production time, and is thus expected to improve annual plant throughput and profitability following implementation at WEST Brewery.

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